Supporting Information for the manuscript "Novel Inorganic-Organic Layered Structures: Crystallographic Understanding ……" by *Zhao-Xiang Deng, Libo Li and Yadong Li**

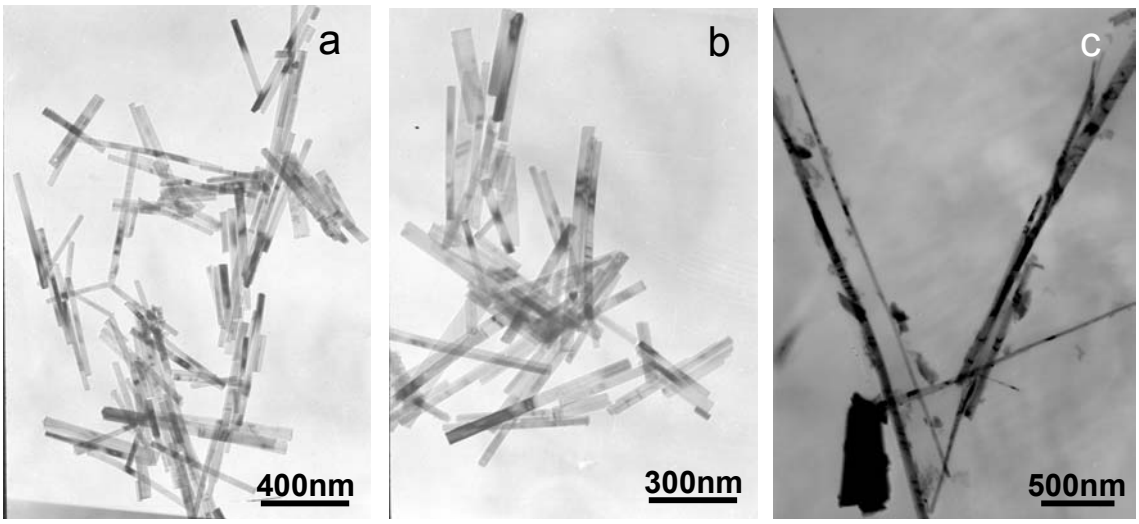

Figure 1. Some TEM pictures of CdS (a, b) and CdSe (c) nanorods synthesized via ethylenediamine-mediated solvothermal route.

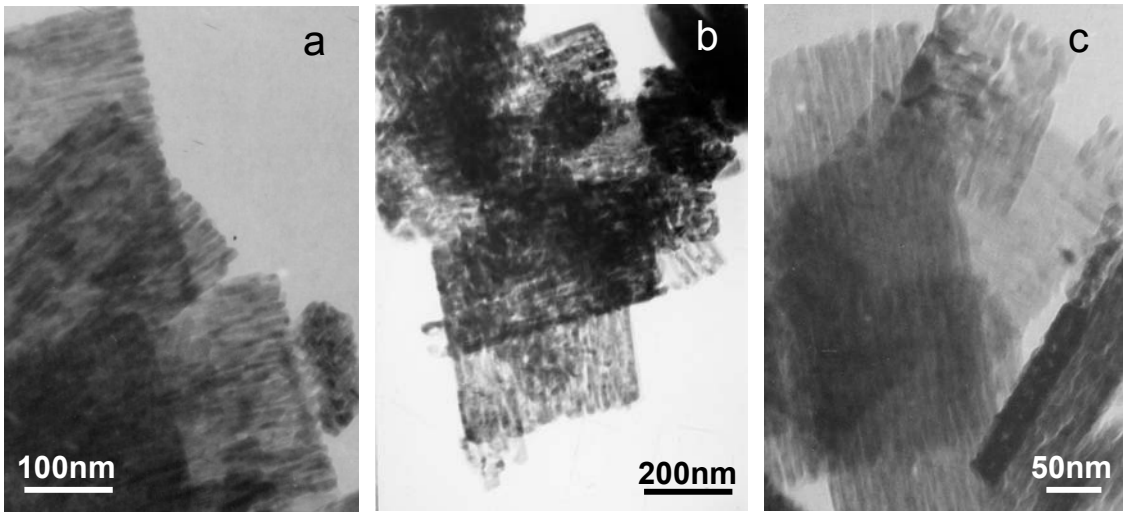

Figure 2. TEM pictures of some striated ZnS (a) and ZnSe (b, c) products synthesized via post thermal processing of the ZnS·0.5en and ZnSe·0.5en precursors.

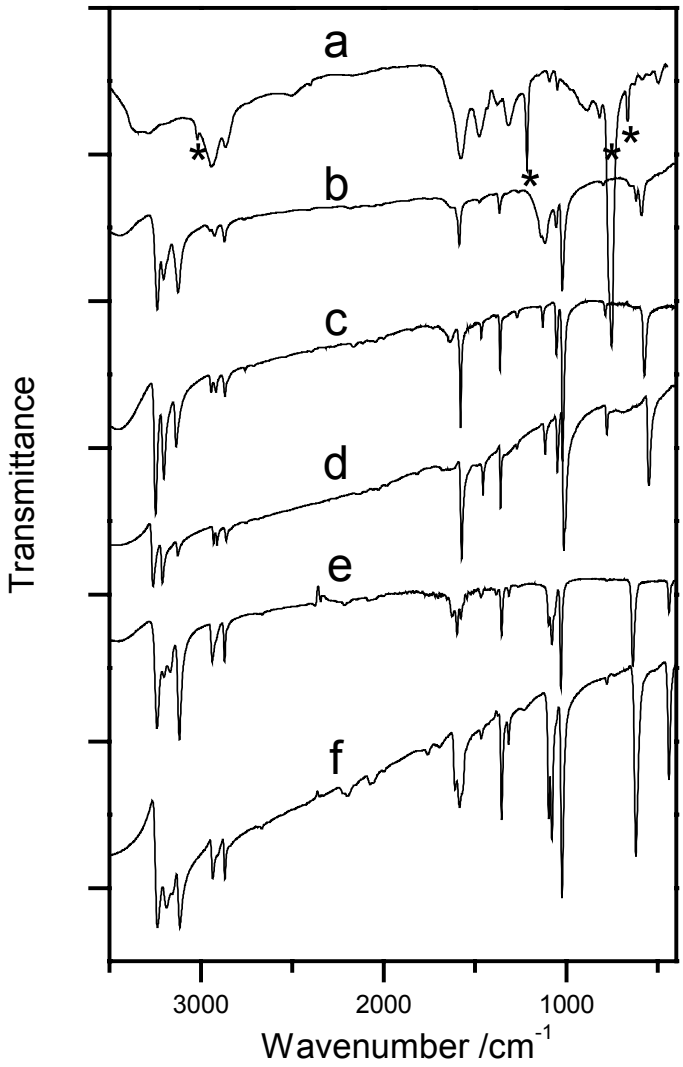

Figure 3. A list of full range IR spectra (400~3500cm^{-1}) of ethylenediamine in chloroform (5% V/V) (a), CdS·0.5en (b), CdSe·0.5en (c), CdTe·0.5en (d), ZnS·0.5en (e) and ZnSe·0.5en (f). Asterisks in curve (a) indicates the vibrations of the solvent chloroform.

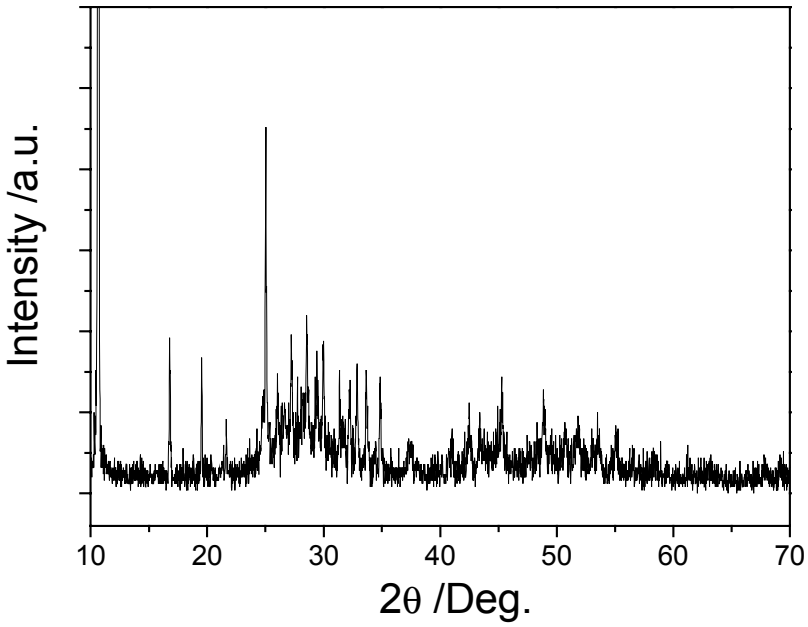

Figure 4. XRD pattern of CdS·0.5en without data-smoothing and background subtraction, showing the existence of unknown amorphous phase.

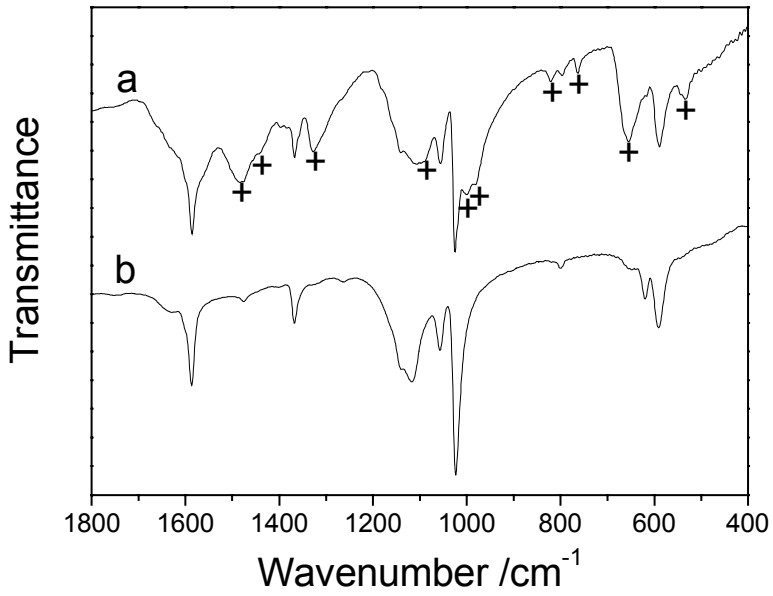

Figure 5. IR spectra of CdS·0.5en before (a) and after (b) drying at 70ºC for 6h. Significant decrease or disappearance of some vibration peaks coming from the adsorbed ethylenediamine molecules could be observed and marked with "+" symbols.

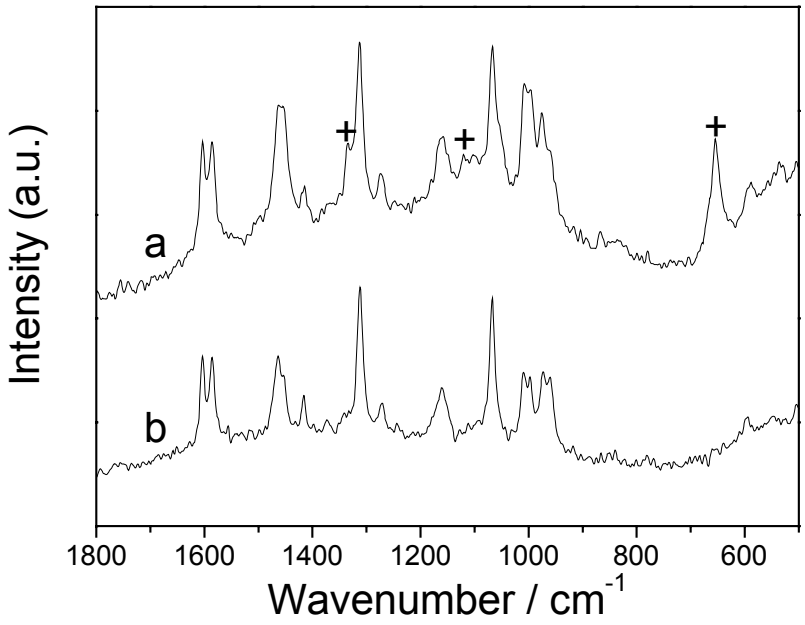

Figure 6. Raman spectra of CdS·0.5en before (a) and after (b) drying at 70ºC for 6h. "+" indicates the peaks corresponding to interface ethylenediamine molecules.

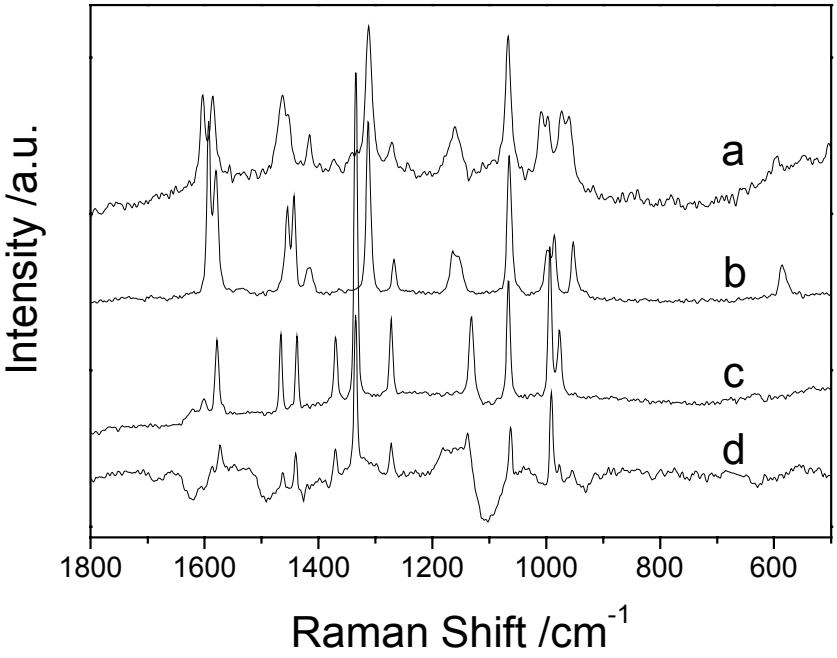

Figure 7. A collection of Raman spectra (500~1800cm^{-1}) of the compounds CdS·0.5en (a), CdSe·0.5en (b), ZnS·0.5en (c) and ZnSe·0.5en (d). The Raman spectrum of ZnSe·0.5en sample had strong fluorescence background, and curve (d) was subtracted from the fluorescence background.

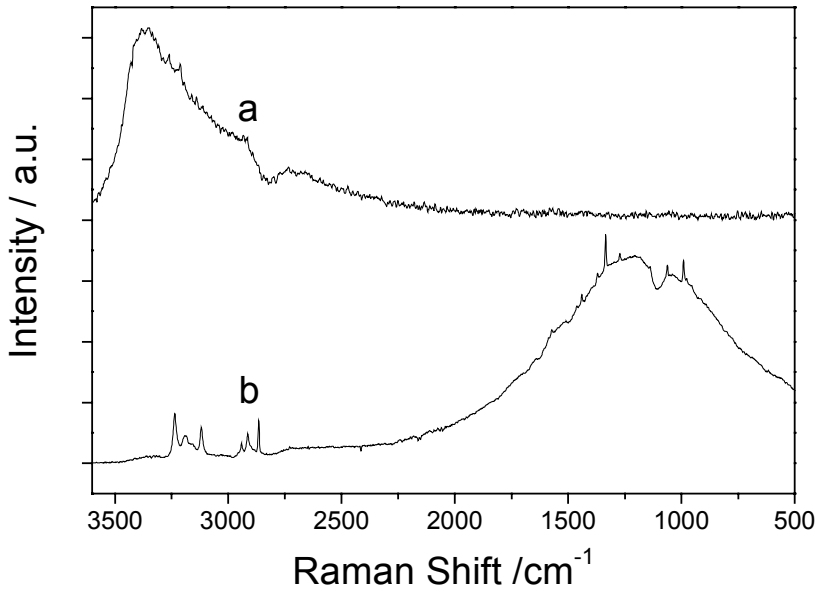

Figure 8. Raman spectra of CdSe·0.5en and ZnSe·0.5en contaminated strongly by broad fluorescence backgrounds.

Table 1. Crystal data and structure refinement for CdSe(en)0.5.

Identification code	CdSe(en)0.5
Empirical formula	C2 H8 Cd2 N2 Se2
Formula weight	442.82
Temperature	296(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P b a c
Unit cell dimensions	a = 7.0848(7) A alpha = 90 deg. b = 6.7856(7) A beta = 90 deg. c = 16.6940(18) A gamma = 90 deg.
Volume	802.56(14) A^3
Z, Calculated density	4, 3.665 Mg/m^3
Absorption coefficient	14.278 mm^-1
F(000)	792
Crystal size	0.1 x 0.05 x 0.02 mm
Theta range for data collection	2.44 to 33.40 deg.
Index ranges	-10<=h<=5, -10<=k<=10, -25<=l<=23
Reflections collected / unique	7027 / 1508 [R(int) = 0.0531]
Completeness to 2theta = 33.40	96.6%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1508 / 0 / 37
Goodness-of-fit on F^2	0.980
Final R indices [I>2sigma(I)]	R1 = 0.0410, wR2 = 0.0740
R indices (all data)	R1 = 0.0576, wR2 = 0.0780
Largest diff. peak and hole	1.545 and -1.394 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 4.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cd(1)	8987(1)	507(1)	6992(1)	21(1)
Se(2)	5556(1)	-732(1)	6681(1)	19(1)
N(3)	10803(6)	-979(7)	5993(3)	22(1)
C(4)	10930(9)	-38(11)	5197(4)	36(2)

Table 3. Bond lengths [A] and angles [deg] for 4.

Cd(1)-N(3)	2.335(5)
Cd(1)-Se(2)#1	2.6173(8)
Cd(1)-Se(2)#2	2.6242(7)
Cd(1)-Se(2)	2.6245(7)
Se(2)-Cd(1)#3	2.6173(8)
Se(2)-Cd(1)#4	2.6242(7)
N(3)-C(4)	1.478(9)
C(4)-C(4)#5	1.474(13)
N(3)-Cd(1)-Se(2)#1	103.39(11)
N(3)-Cd(1)-Se(2)#2	102.16(11)
Se(2)#1-Cd(1)-Se(2)#2	115.32(2)
N(3)-Cd(1)-Se(2)	103.33(12)
Se(2)#1-Cd(1)-Se(2)	117.25(2)
Se(2)#2-Cd(1)-Se(2)	112.75(2)
Cd(1)#3-Se(2)-Cd(1)#4	101.38(2)
Cd(1)#3-Se(2)-Cd(1)	97.05(2)
Cd(1)#4-Se(2)-Cd(1)	99.10(2)
C(4)-N(3)-Cd(1)	119.3(4)
C(4)#5-C(4)-N(3)	111.2(7)

Symmetry transformations used to generate equivalent atoms:
#1 x+1/2,y,-z+3/2 #2 -x+3/2,y+1/2,z
#3 x-1/2,y,-z+3/2 #4 -x+3/2,y-1/2,z
#5 -x+2,-y,-z+1

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 4.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cd(1)	20(1)	21(1)	22(1)	0(1)	0(1)	0(1)
Se(2)	17(1)	18(1)	22(1)	0(1)	0(1)	1(1)
N(3)	22(2)	23(2)	21(3)	7(2)	-2(2)	2(2)
C(4)	27(3)	51(4)	30(4)	1(3)	6(3)	0(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 4.

	x	y	z	U(eq)
H(3A)	11986	-1102	6184	27
H(3B)	10353	-2207	5921	27
H(4A)	11418	1290	5256	44
H(4B)	11803	-773	4864	44